

# Electron correlation vs. stabilization: A two-electron model atom in an intense laser pulse

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We study numerically stabilization against ionization of a fully correlated two-electron model atom in an intense laser pulse. We concentrate on two frequency regimes: very high frequency, where the photon energy exceeds both, the ionization potential of the outer *and* the inner electron, and an intermediate frequency where, from a “single active electron”-point of view the outer electron is expected to stabilize but the inner one is not. Our results reveal that correlation reduces stabilization when compared to results from single active electron-calculations. However, despite this destabilizing effect of electron correlation we still observe a decreasing ionization probability within a certain intensity domain in the high-frequency case. We compare our results from the fully correlated simulations with those from simpler, approximate models. This is useful for future work on “real” more-than-one electron atoms, not yet accessible to numerical *ab initio* methods.

## I. INTRODUCTION

The advent of high intensity lasers led to an increasing interest in non-perturbative studies of atomic systems interacting with intense laser light (see, e.g., [1] for a review). One of the most frequently revisited topics during the last fifteen years was *stabilization* of atoms (or ions) against ionization in intense laser light, i.e., for increasing laser intensity the ionization rate *decreases*. This kind of stabilization was predicted by Gersten and Mittleman already in 1975 [2]. Experimentally, stabilization of highly excited atoms has been reported [3] whereas measuring stabilization of atoms initially in the ground state is hard to achieve. This is due to the fact that, in order to see stabilization, the laser photon energy has to exceed the ionization potential. Unfortunately, there are not yet high intensity lasers available delivering such energetic photons. Therefore most of the studies in this field are of analytical or numerical nature: “high-frequency theory” [4], Floquet calculations [5,6], the numerical treatment of 1D model atoms, quantum [7–10] and classical [11], as well as in two-color laser fields [12], 2D atoms in arbitrary polarized laser light [13], and full 3D hydrogen [14]. Of particular interest is whether the atom survives in a “real” laser pulse up to intensities where stabilization sets in, or whether it already ionizes almost 100% during the rise time of the pulse [15]. In other words: is the atom able to pass through the “death valley” of ionization before arriving at the “magic mountain” of stabilization? There are also several papers where the authors came to the conclusion that stabilization does not exist at all (see [16,17], and references therein).

In this paper we focus on how the electron correlation in a two-electron model atom affects the probability for stabilization, i.e., the probability that the model atom remains neutral after the pulse has passed by. For two frequency regimes we compare the results from the fully correlated calculation with approximate models like “single active electron” or time-dependent density functional theory. The purpose of these studies is, on one hand, to gain a qualitative picture of the stabilization mechanism in a more-than-one electron atom, and, on the other hand, testing approximate methods before applying them to 3D many-electron atoms where accurate, full *ab initio* studies are not possible with current days computers. To our knowledge only a few other numerical studies of correlated two-electron systems in the stabilization regime are reported in the literature so far [18–20].

## II. THE MODEL ATOM

We study a model helium atom where both electrons are allowed to move in one dimension only, but with the electron-electron correlation fully taken into account. This leads to a two-dimensional time-dependent Schrödinger equation (TDSE)

$$i\frac{\partial}{\partial t}|\Psi(t)\rangle = H(t)|\Psi(t)\rangle \quad (1)$$

with the Hamiltonian

$$H(t) = \frac{1}{2}(\mathbf{p}_1 + A(t))^2 + \frac{1}{2}(\mathbf{p}_2 + A(t))^2 - \frac{2}{\sqrt{x_1^2 + \epsilon}} - \frac{2}{\sqrt{x_2^2 + \epsilon}} + \frac{1}{\sqrt{(x_1 - x_2)^2 + \epsilon}}. \quad (2)$$

Here, the laser pulse is coupled to the atom in dipole approximation through the vector potential  $A(t)$ .  $\mathbf{x}_i$  and  $\mathbf{p}_i$  ( $i = 1, 2$ ) are the electrons' coordinates and canonical momenta, respectively. We use atomic units (a.u.) throughout this paper. The regularization parameter  $\epsilon$  was chosen 0.49 which yielded, on our numerical grid, ionization potentials similar to real helium (0.9 a.u. for the first electron, and 2 a.u. for the second one).

The electric field  $E(t) = -\partial_t A(t)$  was a trapezoidal pulse with a rising edge over 5 optical cycles, 5 cycles of constant amplitude  $\hat{E}$ , and a down-ramp over, again, 5 cycles. We started all our simulations with the field-free ground state  $|\Psi(0)\rangle$ . The wavefunction  $\Psi(x_1, x_2, t) = \langle x_1 x_2 | \Psi(t) \rangle$  was propagated in time using an unconditionally stable, explicit “grid hopping” algorithm [21]. Non-vanishing probability amplitude  $\Psi(x_1, x_2)$  near the grid boundary was removed through an imaginary potential. The numerical grid was always several times (at least 10 times) larger than the excursion length

$$\hat{\alpha} = |\hat{E}/\omega^2| = |\hat{A}/\omega| \quad (3)$$

of a classical electron oscillating in the laser field of frequency  $\omega$  and electric field amplitude  $\hat{E}$  (vector potential amplitude  $\hat{A}$ ). During time propagation we monitored the amount of probability density  $|\Psi|^2$  inside a box  $x_1, x_2 \in [-5, +5]$ . After the pulse is over, the density inside this box can be interpreted as the “survival” probability of the helium atom to remain neutral [22].

To analyze the results obtained with this fully correlated model atom we compare with several simplified models. Among those, the “single active electron” (SAE) approximation is the simplest one. There, one assumes that an *inner* and an *outer* electron respond independently to the laser field. The inner electron “feels” the bare nucleus ( $Z_i = 2$ , hydrogen-like). The outer one sees an effective nuclear charge, to be adjusted in such a way that the correct ionization potential (0.9 a.u.) is obtained. In our numerical model this was the case for  $Z_o = 1.1$ . Thus, in the SAE approximation, we solved two independent TDSEs with no dynamic correlation at all,

$$i\partial_t \Psi_i(x, t) = \left( \frac{1}{2}(-i\partial_x + A(t))^2 - \frac{Z_i}{\sqrt{x^2 + \epsilon}} \right) \Psi_i(x, t), \quad (4)$$

$$i\partial_t \Psi_o(x, t) = \left( \frac{1}{2}(-i\partial_x + A(t))^2 - \frac{Z_o}{\sqrt{x^2 + \epsilon}} \right) \Psi_o(x, t). \quad (5)$$

In order to incorporate correlation in a first step one can introduce a Hartree-type potential into the Hamiltonian for the inner electron,

$$i\partial_t \Psi_i(x, t) = \left( \frac{1}{2}(-i\partial_x + A(t))^2 - \frac{Z_i}{\sqrt{x^2 + \epsilon}} + \int \frac{|\Psi_o(x', t)|^2}{\sqrt{(x - x')^2 + \epsilon}} dx' \right) \Psi_i(x, t), \quad (6)$$

$$i\partial_t \Psi_o(x, t) = \left( \frac{1}{2}(-i\partial_x + A(t))^2 - \frac{Z_o}{\sqrt{x^2 + \epsilon}} \right) \Psi_o(x, t). \quad (7)$$

In this approximation, the inner electron feels the bare nuclear potential *and* the outer electron. Therefore, we call this model “inner sees outer” (ISO) approximation. It was utilized in Ref. [23] to study non-sequential ionization (NSI). In the ground state, the Hartree-potential leads to a screening of the bare nuclear charge. Thus, energetically the two electrons are almost equivalent in the beginning, though we labelled them “inner” and “outer” in Eqs. (6), (7). However, during the interaction with the laser field one of the electrons might become the outer one. We will also consider the opposite point of view where the outer electron sees the inner one (“outer sees inner”, OSI). In this case we have to deal with the system of TDSEs

$$i\partial_t \Psi_i(x, t) = \left( \frac{1}{2}(-i\partial_x + A(t))^2 - \frac{Z}{\sqrt{x^2 + \epsilon}} \right) \Psi_i(x, t), \quad (8)$$

$$i\partial_t \Psi_o(x, t) = \left( \frac{1}{2}(-i\partial_x + A(t))^2 - \frac{Z}{\sqrt{x^2 + \epsilon}} + \int \frac{|\Psi_i(x', t)|^2}{\sqrt{(x - x')^2 + \epsilon}} dx' \right) \Psi_o(x, t). \quad (9)$$

with  $Z = 2$ .

Finally, another way to study our model system is to apply time-dependent density functional theory (TDDFT) (see [24] for an overview) in local density approximation, leading to the (nonlinear) TDSE for *one* Kohn-Sham orbital  $\Phi(x, t)$ ,

$$i\partial_t\Phi(x, t) = \left( \frac{1}{2}(-i\partial_x + A(t))^2 - \frac{2}{\sqrt{x^2 + \epsilon}} + \int \frac{|\Phi(x', t)|^2}{\sqrt{(x - x')^2 + \epsilon}} dx' \right) \Phi(x, t). \quad (10)$$

The total electron probability density is given by  $n(x, t) = 2|\Phi(x, t)|^2$ . Since, strictly speaking,  $\Phi(x, t)$  cannot be interpreted as a physically meaningful single electron orbital it is not easy to deduce single electron quantities (such as single ionization for instance). On the other hand, the somewhat arbitrary distinction between an inner and an outer electron is avoided in TDDFT.

### III. HIGH-FREQUENCY RESULTS

#### A. Single active electron-approximation

In this Section we want to compare the results from the fully correlated model atom with those from the corresponding SAE calculations. First, we focus on the high-frequency regime where the laser frequency exceeds both ionization potentials,  $\omega = \pi > \mathcal{E}_i > \mathcal{E}_o$ . From an SAE-point of view we expect both electrons to stabilize, especially the outer one since the frequency is 3.5 times larger than the ionization potential  $\mathcal{E}_o = 0.9$ . In Fig. 1 the amount of probability density inside the box  $x_1, x_2 \in [-5, +5]$  (PDIB) vs. time for  $\hat{\alpha} = 0.5, 1.0, 1.5$  and  $2.0$  is shown for the inner and the outer electron. First we observe the expected result that the outer electron is more stabilized than the inner one: the amount of PDIB after the pulse has gone is greater for the outer electron. However, qualitatively the set of curves are quite similar. For the two higher  $\hat{\alpha}$ -values (1.5, drawn dashed, and 2.0, drawn dashed-dotted) one observes that the curves bend sharply after the up-ramping at  $t = 5$  cycles, i.e., for both electrons ionization is much slower during the constant, intense part of the pulse. In fact, ionization happens almost exclusively during the rampings. We also note that the slight decrease of the PDIB during the constant part of the  $\hat{\alpha} = 1.5$  and  $\hat{\alpha} = 2.0$ -pulses is linear in time, in contrast to tunneling ionization where we have an exponential dependence (in the case of a constant ionization rate). Approximately two cycles after the down-ramping at  $t = 10$  cycles, ionization starts to increase again. Finally, after the pulse is over (at  $t = 15$  cycles) the amount of PDIB remains stationary. Secondly, we observe that there is obviously no monotonous behavior of stabilization with increasing intensity (or  $\hat{\alpha}$ ). Ionization is higher for  $\hat{\alpha} = 1.0$  (dotted curves) than for  $\hat{\alpha} = 0.5$  (solid curves). For  $\hat{\alpha} = 1.5$  (dashed curves) ionization starts to decrease, i.e., we are entering the stabilization domain at that point. Therefore the so-called “death valley” seems to be located around  $\hat{\alpha} = 1$  for *both* electrons in our model atom.

In Fig. 2 the stabilization probability for both electrons is shown vs. the excursion  $\hat{\alpha}$ . The quiver amplitude  $\hat{\alpha}$  is related to the laser intensity  $I = \hat{E}^2$  through  $\hat{\alpha} = I^{1/2}\omega^{-2}$ . The stabilization probability of the inner electron exhibits an oscillatory behavior. The “death valley” is located at  $\hat{\alpha} \approx 1$ , followed by a maximum at  $\hat{\alpha} \approx 4$ . For higher intensity ionization increases again up to a stabilization minimum around  $\hat{\alpha} \approx 7$ . Stabilization of the inner electron recovers till the next maximum at  $\hat{\alpha} \approx 9$ . The second maximum is below the first. Thus we observe an overall decrease of stabilization with increasing intensity. This is even more pronounced in the stabilization probability for the outer electron where the oscillations are less visible. The “death valley” for both electrons is located at  $\hat{\alpha} \approx 1$  while the maxima are at different positions. The oscillatory character of the stabilization probability in 1D systems has been observed by other authors as well [25–27]. In contrast to our results an overall increase of stabilization with increasing intensity was found in [25,26]. This might be due to the fact that we are looking at the ionization *probability* after the pulse is over while in analytical papers often the ionization *rate* is discussed. In the former, ionization during the up and down-ramps is taken into account while in the latter it is commonly not.

The probability for our He model atom to survive as neutral He after the pulse is over is, in SAE approximation, simply the product of the probabilities for each electron to remain bound. In Fig. 2 the corresponding curve is indicated by i-o. The result from the fully correlated system is also shown (drawn dotted, indicated with ‘corr’). We infer that, especially for  $\hat{\alpha} < 5$  the stabilization probability is strongly overestimated by the SAE treatment. We could argue that *if* the system stabilizes it will probably stabilize in such a way that the correlation energy is minimized. In that case it sounds more reasonable to take the square of the SAE stabilization probability for the *inner* electron. In what follows we will refer to this viewpoint as “independent electron” (IE) model since it follows from crossing out the correlation term in the Hamiltonian (2). The result is included in Fig. 2, labelled i-i. The IE-curve seems to oscillate around the fully correlated one, especially for  $\hat{\alpha} > 6$ . From this result we conclude that, compared to the IE-model

with two equivalent inner electrons, electron correlation washes out oscillations in the stabilization probability and, therefore, can stabilize as well as destabilize, depending on the intensity (for a given pulse shape and frequency).

To discuss that further we look at the time-averaged Kramers-Henneberger potential (TAKHP), i.e., we transform to the frame of reference where the quivering electron is at rest but the nuclear potential oscillates, and average over one cycle,

$$V_{KH}^{corr}(x_1, x_2) = \sum_{i=1}^2 \frac{\omega}{2\pi} \int_0^{2\pi/\omega} \frac{-2}{\sqrt{(x_i + \alpha(t))^2 + 0.49}} dt + \frac{1}{\sqrt{(x_1 - x_2)^2 + 0.49}}. \quad (11)$$

For sufficiently high frequencies this is the leading term in a perturbation series in  $\omega^{-1}$  [4]. In the correlation term no  $\alpha(t)$  appears since the interparticle distance is not affected by the KH transformation. We calculated numerically the TAKHP. The result is shown in Fig. 3 for  $\alpha(t) = \hat{\alpha} \sin \omega t$  with  $\hat{\alpha} = 5$ . For comparison the TAKHP with the correlation term neglected is also shown (corresponding to the IE model). With correlation, there are two minima near  $x_1 = \hat{\alpha}, x_2 = -\hat{\alpha}$  and  $x_1 = -\hat{\alpha}, x_2 = \hat{\alpha}$  whereas without correlation there are two more, energetically equivalent minima at  $x_1 = x_2 = \hat{\alpha}$  and  $x_1 = x_2 = -\hat{\alpha}$ . However, if we assume that the fully correlated system manages it *somehow* to occupy the ground state of  $V_{KH}^{corr}$ , the correlation energy will be small (for not too small  $\hat{\alpha}$ ) since the interparticle distance is  $2\hat{\alpha}$ . The higher  $\hat{\alpha}$  the lower the correlation energy. We believe that this is the physical reason that, for increasing  $\hat{\alpha}$ , the agreement of the IE results with the fully correlated ones becomes quite good (although the latter do not exhibit an oscillating stabilization probability). Our viewpoint is further supported by examining the probability density of the fully correlated system during the pulse. In Fig. 4  $|\Psi(x_1, x_2)|^2$  is shown for  $\omega = \pi$ ,  $\hat{\alpha} = 4.0$  at  $t = 7.5$  cycles, i.e., in the middle of the constant part of the trapezoidal pulse. We clearly observe *dichotomy*, i.e., two probability density peaks at the classical turning points, well known from one-electron systems [4]. Due to electron correlation we do not observe four peaks. Instead the peaks at  $x_1 = x_2 = \pm 4$  are suppressed, in accordance with our discussion of the TAKHPs in Fig. 3. Therefore the correlation energy is rather small since the distance between the two peaks in the  $x_1 x_2$ -plane is  $\sqrt{8}\hat{\alpha}$ . In the work by Mittleman [28] such multi-electron “dichotomized” bound states are calculated.

## B. Time-dependent density functional theory

In Fig. 5 our results from the TDDFT calculations are presented. Although the Kohn-Sham orbital  $\Phi(x, t)$  is an auxiliary entity that has, in a rigorous sense, no physical meaning, we take it as an approximation to a single electron orbital. If we do this,  $|\Phi(x, t)|^2 \cdot |\Phi(x, t)|^2$ , integrated over the region  $-5 < x < 5$  after the pulse is over, is our TDDFT stabilization probability. We see that for  $\hat{\alpha} < 1.5$  the agreement between TDDFT and correct result is very good. The difference between TDDFT and IE (indicated by i-i again) is a direct measure of correlation effects since both models differ by the Hartree-term in the Hamiltonian only. Up to  $\hat{\alpha} \approx 5.5$  electron correlation suppresses stabilization compared to the IE approximation. In that region TDDFT agrees better with the full result. As mentioned before, for higher  $\hat{\alpha}$  the IE curve oscillates around the correct result and therefore it comes occasionally to a very good agreement with the exact result. Also the TDDFT result agrees very well with the fully correlated curve for  $\hat{\alpha} \geq 7$ . In summary we can say that the TDDFT result is in good agreement with the exact, fully correlated stabilization probability. Both have their maximum around  $\hat{\alpha} \approx 4$  and the “death valley” is also at the right position. For higher  $\hat{\alpha}$  the agreement seems to become even better.

## C. “Inner sees outer” and “outer sees inner”-approximation

In order to explain non-sequential ionization (NSI; see, e.g., Ref. [1] for an overview) it is essential to incorporate electron correlation (see [29] for a very recent paper, and references therein). For that purpose Watson *et al.* [23] added a Hartree-type potential to the TDSE for the inner electron (see Eq. 6, ISO). By doing this the double ionization yield is greatly enhanced, in accordance with experimental results [30]. The question we address in this Section is whether this method is applicable to stabilization as well. We will also study the opposite procedure, i.e., where the outer electron feels the inner one (see Eqs. 8 and 9, OSI). From the discussions on the SAE approximation above we can expect that ISO will probably not agree very well with the exact results since the assumption that the outer electron sees a static, effective nuclear charge is not valid. In Fig. 6 we see that, for low  $\hat{\alpha}$  ISO ( $\triangle$ ) behaves like SAE (the i-o-curve) while OSI ( $\diamond$ ) is similar to IE (the curve indicated by i-i). In ISO approximation for  $\hat{\alpha} > 3$  the electron correlation obviously causes strong ionization, compared to the SAE result. Especially during the down-ramping, when probability density of the outer electron moves from the turning points  $\pm \hat{\alpha}$  back toward the nucleus, ionization

of the inner electron is enhanced. For  $\hat{\alpha} > 4.5$  the ISO curve even drops below the exact result (indicated by ‘corr’). In OSI approximation the stabilization probability is also underestimated for  $\hat{\alpha} > 4.5$ . In summary we can say, that for  $\hat{\alpha} < 2$ , OSI is in very good agreement with the correct result while ISO is not, due to the inappropriate assumption of the outer electron feeling just a static effective nuclear charge. However, for higher  $\hat{\alpha}$  ISO and OSI tend to underestimate the stabilization probability while TDDFT does not (see Section III B and Fig. 5).

#### IV. INTERMEDIATE FREQUENCY RESULTS

In this Section we discuss the stabilization probability in the intermediate frequency regime  $\mathcal{E}_o < \omega < \mathcal{E}_i$  where, according a single active electron point-of-view, the outer electron should stabilize while for the inner one ionization is more likely. In Fig. 7 we compare the result from the fully correlated calculation with those from the SAE treatment. In SAE approximation, the outer electron is more stable than the inner one in the region  $1.5 < \hat{\alpha} < 8.5$ . For the inner electron no clear stabilization maximum is visible. For the outer electron the maximum is at  $\hat{\alpha} \approx 6$ , i.e., it is shifted toward higher  $\hat{\alpha}$  compared to the high-frequency case. Both, i-o and i-i underestimates ionization, especially for low  $\hat{\alpha}$  in the “death valley”-region. Electron correlation obviously enhances ionization. For lower frequencies this is the well-known effect of NSI ([29] and references therein). Although in the fully correlated result we observe a stabilization probability maximum around  $\hat{\alpha} \approx 7.5$  the absolute value is below 0.04, and, in our opinion, it makes no sense to talk about real “stabilization” in that case. As in the high-frequency-case we observe an overall decrease of the stabilization probability for very high  $\hat{\alpha}$ -values.

In Fig. 8 we compare the result from the fully correlated model atom with the corresponding ones from the ISO, OSI, and TDDFT runs where electron correlation is included approximately. Let us first focus on the  $\hat{\alpha}$ -region “left from the death valley”, i.e.,  $\hat{\alpha} \leq 1$ . There we observe that ISO is nearest to the correct result while OSI and TDDFT underestimates ionization. This is quite understandable within the present knowledge of how NSI works: the inner electron needs to interact with laser field *and* the outer electron in order to become free. Obviously this is best accounted for in the ISO approximation. For most  $\hat{\alpha}$  TDDFT lies between the ISO and the OSI result. This is also quite clear since in TDDFT both correlated electrons are treated on an equal footing (one Kohn-Sham-orbital only) whereas in ISO (OSI) the inner (outer) electron feels the outer (inner) partner through Coulomb correlation, but not vice versa. However, all these approximations still overestimate the stabilization probability, at least in the interesting  $\hat{\alpha}$ -regime where the stabilization probability rises at all (i.e., for  $2 < \hat{\alpha} < 7.5$ ).

To summarize this Section we can say that in order to achieve stabilization of our two-electron model atom it is necessary to choose a laser frequency that exceeds *all* ionization potentials. For an intermediate frequency the outer electron cannot stabilize owing to correlation. The SAE picture is not appropriate and even ISO, OSI, or TDDFT where electron correlation is included approximately fail.

#### V. DISCUSSION AND SUMMARY

In this paper we studied how the electron correlation in a two-electron model atom affects the probability for stabilization. We found clear stabilization only for frequencies that exceed *both* ionization potentials. Although for the intermediate frequency we did not find a monotonous increase of the ionization probability with increasing intensity we prefer not calling this effect stabilization since, on an absolute scale, its probability was very small. In all cases electron correlation reduced the stabilization probability compared to the SAE picture. In the high-frequency case the two electrons behave more like two independent *inner* electrons. Similar results were obtained by Grobe and Eberly [18] for a  $H^-$  model-ion. Lewenstein *et al.* [19] performed classical calculations for a model-atom similar to ours which also showed that “dichotomized” two-electron states are dynamically accessible.

The agreement of the exact numerical result with TDDFT in the high-frequency case was quite good while in the intermediate frequency regime stabilization was overestimated by *all* approximate techniques (ISO, OSI, and TDDFT).

It is well-known that a slow time-scale in the stabilization dynamics is introduced owing to floppings between states in the time-averaged Kramers-Henneberger potential [4,10]. It can be easily imagined that these slow floppings are affected by electron correlation because, e.g., the merging of the two dichotomous peaks into a single one is suppressed then. But even without correlation the results for the stabilization probability are quite sensitive to rise time and pulse duration of the laser field since it strongly depends on which Kramers-Henneberger states are mainly occupied at the time instant when the laser pulse ends. To avoid these additional complications in the interpretation of the numerical results we chose a rather short laser pulse duration so that low-frequency Rabi-floppings do not play a

role. Therefore, in the high-frequency studies we just observed the two dichotomous peaks building up (as depicted in Fig. 4) but no peak-merging during the constant part of our trapezoidal laser pulse.

Finally, we would like to comment on the reduced dimensionality of our two-electron model atom. We also performed calculations with “real”, i.e., three-dimensional (3D) hydrogen-like ions in the stabilization regime. It seems to be the case that in 3D stabilization is less pronounced. Moreover, the oscillatory character is less visible, i.e., we observe a single stabilization maximum followed by a rather monotonous increase of the ionization probability. The difference of 1D models and 3D hydrogen was also studied in Ref. [26]. The effect of electron correlation in 3D stabilization will be the subject of a future paper [31].

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- \* <http://www.physik.tu-darmstadt.de/tqe/>
- [1] M. Protopapas, C. H. Keitel, and P. L. Knight, Rep. Progr. Phys. **60**, 389 (1997).
  - [2] J. I. Gersten and M. H. Mittleman, Phys. Rev. A **11**, 1103 (1975).
  - [3] M. P. de Boer, J. H. Hoogenraad, R. B. Vrijen, L. D. Noordam, and H. G. Muller, Phys. Rev. Lett. **71**, 3263 (1993); M. P. de Boer, J. H. Hoogenraad, R. B. Vrijen, and L. D. Noordam, Phys. Rev. A **50**, 4133 (1994); N. J. van Druten, R. C. Constantinescu, J. M. Schins, H. Nieuwenhuize, and H. G. Muller, Phys. Rev. A **55**, 622 (1997).
  - [4] M. Gavrilă in: *Atoms in Intense Laser Fields* ed. by M. Gavrilă (Academic, New York, 1992), p. 435, and references therein.
  - [5] Martin Dörr, R. M. Potvliege, Daniel Proulx, and Robin Shakeshaft, Phys. Rev. A **43**, 3729 (1991).
  - [6] F. H. M. Faisal, L. Dimou, H.-J. Stiemke, M. Nurhuda, Journ. of Nonl. Opt. Phys. and Materials **4**, 701 (1995).
  - [7] Q. Su, J. H. Eberly, and J. Javanainen, Phys. Rev. Lett. **64**, 862 (1990).
  - [8] R. Grobe and J. H. Eberly, Phys. Rev. Lett. **68**, 2905 (1992).
  - [9] R. Grobe and J. H. Eberly, Phys. Rev. A **47**, R1605 (1993).
  - [10] R. M. A. Vivirito and P. L. Knight, J. Phys. B: At. Mol. Opt. Phys. **28**, 4357 (1995).
  - [11] A. T. Rosenberger, C. C. Sung, S. D. Pethel, and C. M. Bowden, Phys. Rev. A **56**, 2459 (1997).
  - [12] Taiwang Chen, Jie Liu, and Shigang Chen, Phys. Rev. A **59**, 1451 (1999).
  - [13] A. Patel, M. Protopapas, D. G. Lappas, and P. L. Knight, Phys. Rev. A **58**, R2652 (1998).
  - [14] Kenneth C. Kulander, Kenneth J. Schafer, and Jeffrey L. Krause, Phys. Rev. Lett. **66**, 2601 (1991).
  - [15] P. Lambropoulos, Phys. Rev. Lett. **55**, 2141 (1985).
  - [16] A. Fring, V. Kostykin, and R. Schrader, J. Phys. B: At. Mol. Opt. Phys. **29**, 5651 (1996).
  - [17] S. Geltman, J. Phys. B: At. Mol. Opt. Phys. **32**, 853 (1999).
  - [18] R. Grobe and J. H. Eberly, Phys. Rev. A **47**, R1605 (1993).
  - [19] Maciej Lewenstein, Kazimierz Rzążewski, and Pascal Salières, in *Super-Intense Laser-Atom Physics*, ed. by B. Piraux et al., (Plenum, New York, 1993), p. 425.
  - [20] E. A. Volkova, A. M. Popov, and O. V. Tikhonova, JETP **87**, 875 (1998); [Zh. Eksp. Teor. Fiz. **114**, 1618 (1998)] .
  - [21] Hans DeRaedt, Comp. Phys. Rep. **7**, 1 (1987).
  - [22] The atom might be in an excited state after the pulse is over. In order to check this and allow for autoionization we continued the calculation for another 10 atomic time units (for  $\omega = \pi$ ) or 20 a.u. (for  $\omega = \pi/2$ ).
  - [23] J. B. Watson, A. Sanpera, D. G. Lappas, P. L. Knight, and K. Burnett, Phys. Rev. Lett. **78**, 1884 (1997).
  - [24] E. K. U. Gross, J. F. Dobson, and M. Petersilka, in *Topics in Current Chemistry, Vol. 181* (Springer, Berlin, 1996), p. 81.
  - [25] Guanhua Yao and Shih-I Chu, Phys. Rev. A **45**, 6735 (1992).
  - [26] Thomas Millack, J. Phys. B: At. Mol. Opt. Phys. **26**, 4777 (1993).
  - [27] Q. Su, B. P. Irving, C. W. Johnson, and J. H. Eberly, J. Phys. B: At. Mol. Opt. Phys. **29**, 5755 (1996).
  - [28] Marvin H. Mittleman, Phys. Rev. A **42**, 5645 (1990).
  - [29] A. Becker and F. H. M. Faisal, Phys. Rev. A **59**, R1742 (1999).
  - [30] B. Walker, B. Sheehy, L. F. DiMauro, P. Agostini, K. J. Schafer, and K. C. Kulander, Phys. Rev. Lett. **73**, 1227 (1994).
  - [31] F. Ceccherini, D. Bauer, and P. Mulser, to be submitted.

FIG. 1. The amount of probability density inside the box  $x_1, x_2 \in [-5, +5]$  vs. time for  $\hat{\alpha} = 0.5, 1.0, 1.5$  and  $2.0$  (drawn solid, dotted, dashed, and dashed-dotted, respectively) for the inner and the outer electron in “single active electron”-approximation. The laser pulse of frequency  $\omega = \pi$  was ramped-up linearly (in field) over 5 cycles, held constant for another 5 cycles before the linear down-ramp between  $t = 10$  and  $t = 15$  cyc. As expected, the outer electron is more stabilized. For the two higher  $\hat{\alpha}$ -values we clearly see that ionization is weak during the *intense, constant* part of the pulse.

FIG. 2. Stabilization probability for inner (i) and outer (o) electron in SAE-approximation for  $\omega = \pi$ . The fully correlated treatment leads to the stabilization probability (i.e., the probability for the He model atom to survive as *neutral* He) drawn dotted and indicated with ‘corr’. From a SAE viewpoint one would expect the product of the curves i and o, indicated with ‘i-o’. Obviously, in SAE approximation the stabilization probability is overestimated. The so-called “death valley” (dv) for small  $\hat{\alpha}$  is located around  $\hat{\alpha} \approx 1$  for both, SAE and fully correlated results. The i-i-curve results from an independent electron model with two inner electrons. This curve seems to oscillate around the correct curve ‘corr’.

FIG. 3. The time-averaged Kramers-Henneberger potential with ( $V_{KH}^{corr}$ ) and without ( $V_{KH}$ ) electron correlation included for  $\hat{\alpha} = 5$ . With correlation, there are two minima near  $x_1 = \hat{\alpha}, x_2 = -\hat{\alpha}$  and  $x_1 = -\hat{\alpha}, x_2 = \hat{\alpha}$  whereas without correlation there are two more, energetically equivalent minima at  $x_1 = x_2 = \hat{\alpha}$  and  $x_1 = x_2 = -\hat{\alpha}$ . However, once the fully correlated system is in the ground state corresponding to  $V_{KH}^{corr}$ , the correlation energy is small (for not too small  $\hat{\alpha}$ ) since the interparticle distance is  $2\hat{\alpha}$ .

FIG. 4. Probability density  $|\Psi(x_1, x_2)|^2$  for  $\omega = \pi$ ,  $\hat{\alpha} = 4.0$  at  $t = 7.5$  cycles, i.e., in the middle of the constant part of the trapezoidal pulse. We clearly observe *dichotomy*, i.e., two probability density peaks around  $x_1 = \mp 4, x_2 = \pm 4$ . Therefore the correlation energy is rather small since the distance between the two peaks in the  $x_1 x_2$ -plane is  $\sqrt{8}\hat{\alpha}$ .

FIG. 5. Stabilization probability in the high-frequency case ( $\omega = \pi$ ) calculated from time-dependent density functional theory (TDDFT). The fully correlated results (labelled ‘corr’) and the independent electron curve (indicated by i-i) are included for comparison. The agreement of TDDFT with the exact result is good: “death valley” and stabilization maximum are at the same  $\hat{\alpha}$  position. For higher  $\hat{\alpha}$  the agreement is even better.

FIG. 6. Comparison of “inner sees outer” (ISO,  $\triangle$ ) and “outer sees inner” (OSI,  $\diamond$ ) results with the fully correlated ones (corr). Also shown are the “single active electron” (SAE) stabilization probability (i-o) and the “independent electron” (IE) prediction (i-i), already presented in Fig. 2 and discussed in Section III A. For low  $\hat{\alpha}$  ISO behaves like SAE while OSI agrees with IE. For  $\hat{\alpha} > 4.5$  the ISO curve drops below the exact result. In OSI approximation the stabilization probability is also underestimated for  $\hat{\alpha} > 4.5$ .

FIG. 7. Stabilization probability for inner (i) and outer (o) electron in SAE-approximation for the intermediate frequency  $\omega = \pi/2$ . The fully correlated treatment leads to the stabilization probability drawn dotted and indicated with ‘corr’. From a SAE viewpoint one would expect the product of the curves i and o, indicated with ‘i-o’. The i-i-curve results from an independent electron model with two inner electrons. All these models underestimate ionization, i.e., they overestimate stabilization (please note that the stabilization probability is on a logarithmic scale now).

FIG. 8. Comparison of “inner sees outer” (ISO,  $\triangle$ ), “outer sees inner” (OSI,  $\diamond$ ), and time-dependent density functional theory (TDDFT, +) results with the fully correlated ones (corr). Stabilization is overestimated in the ISO, OSI, or TDDFT approximation.

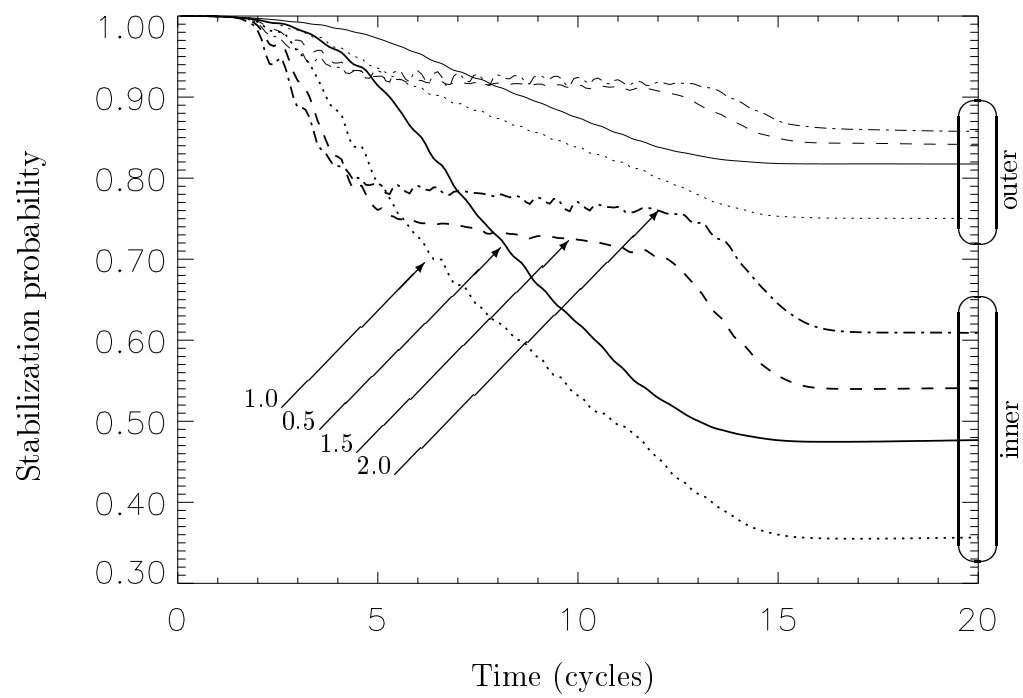


Fig. 1: Bauer and Ceccherini, “Electron correlation vs. ...”



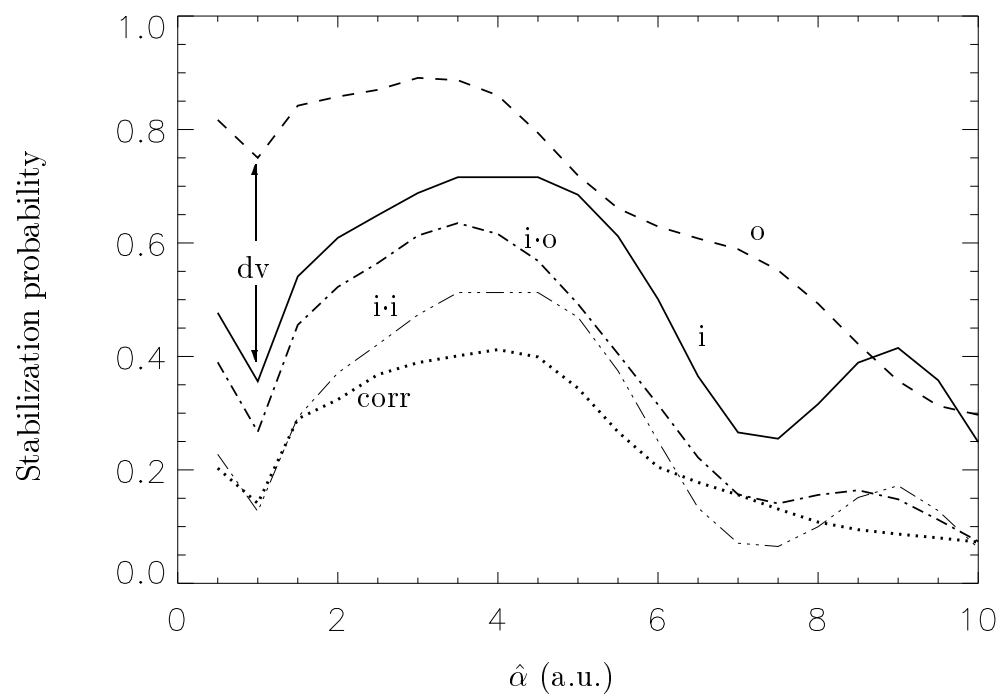


Fig. 2: Bauer and Ceccherini, “Electron correlation vs. ...”

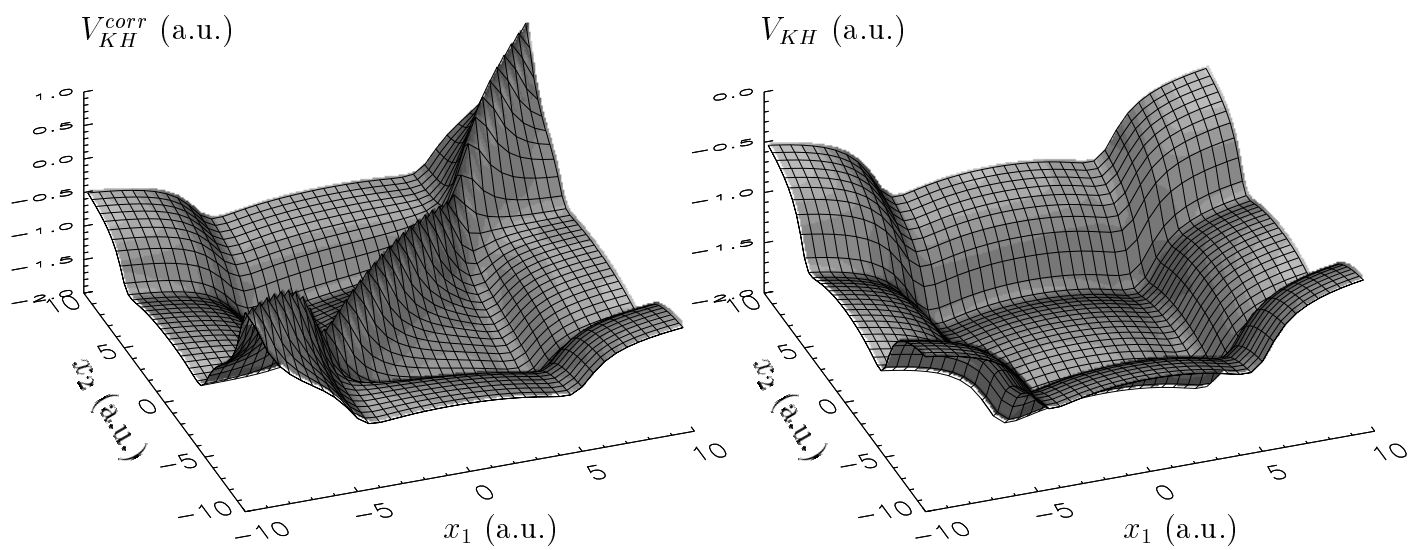


Fig. 3: Bauer and Ceccherini, “Electron correlation vs. ...”

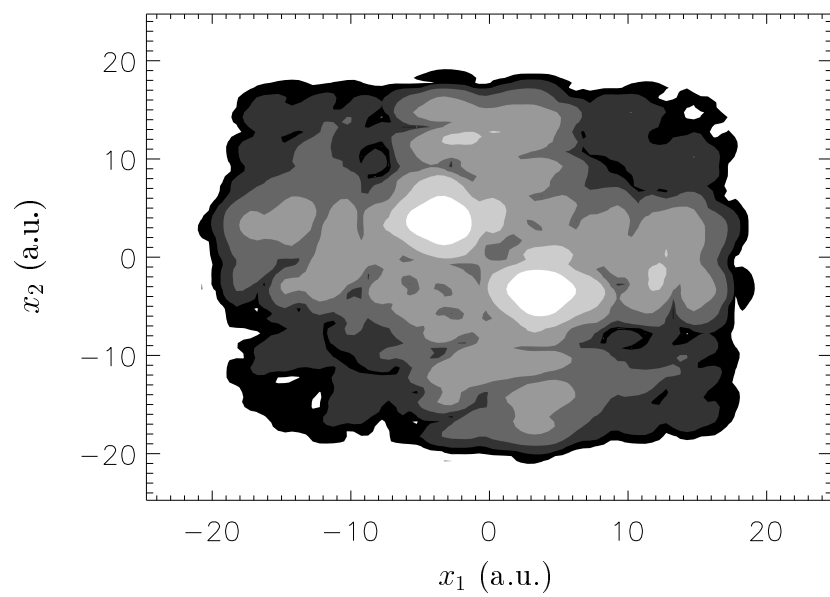


Fig. 4: Bauer and Ceccherini, “Electron correlation vs. ...”

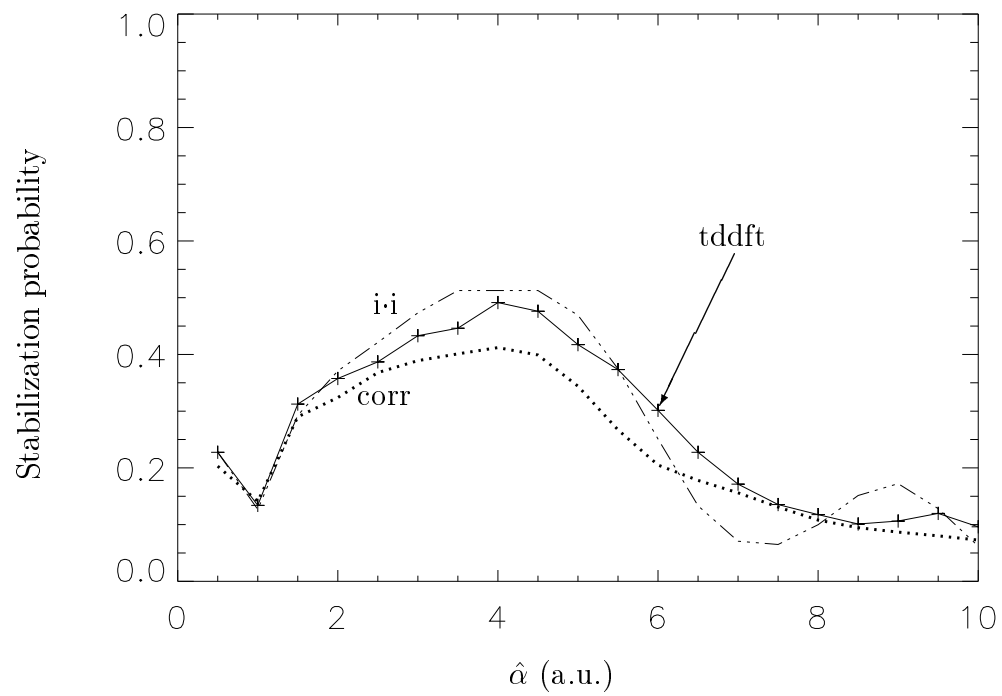


Fig. 5: Bauer and Ceccherini, “Electron correlation vs. ...”

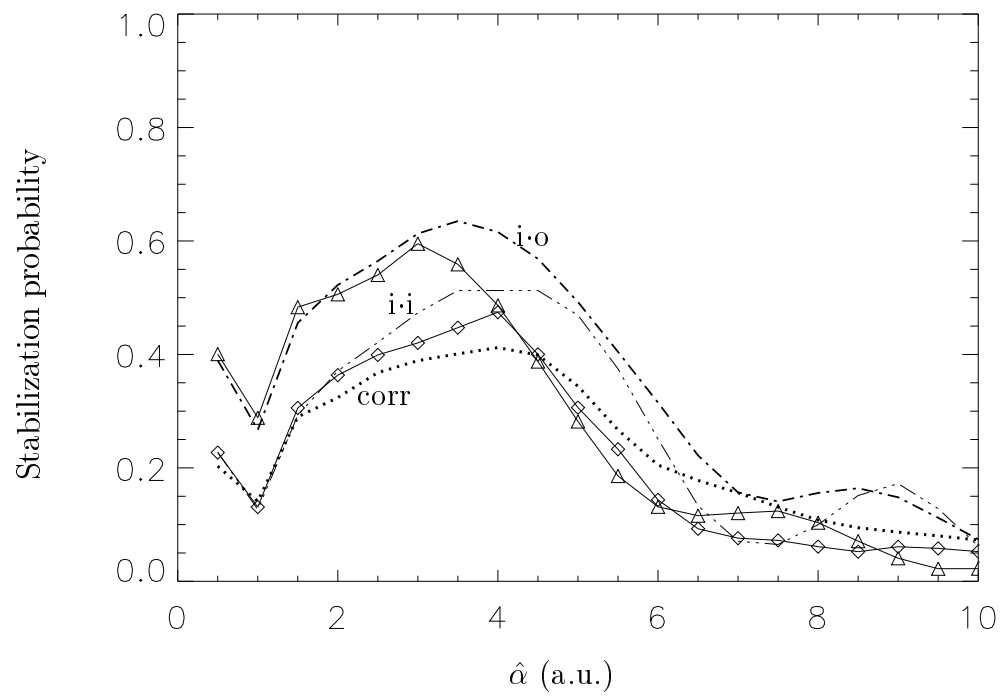


Fig. 6: Bauer and Ceccherini, “Electron correlation vs. ...”

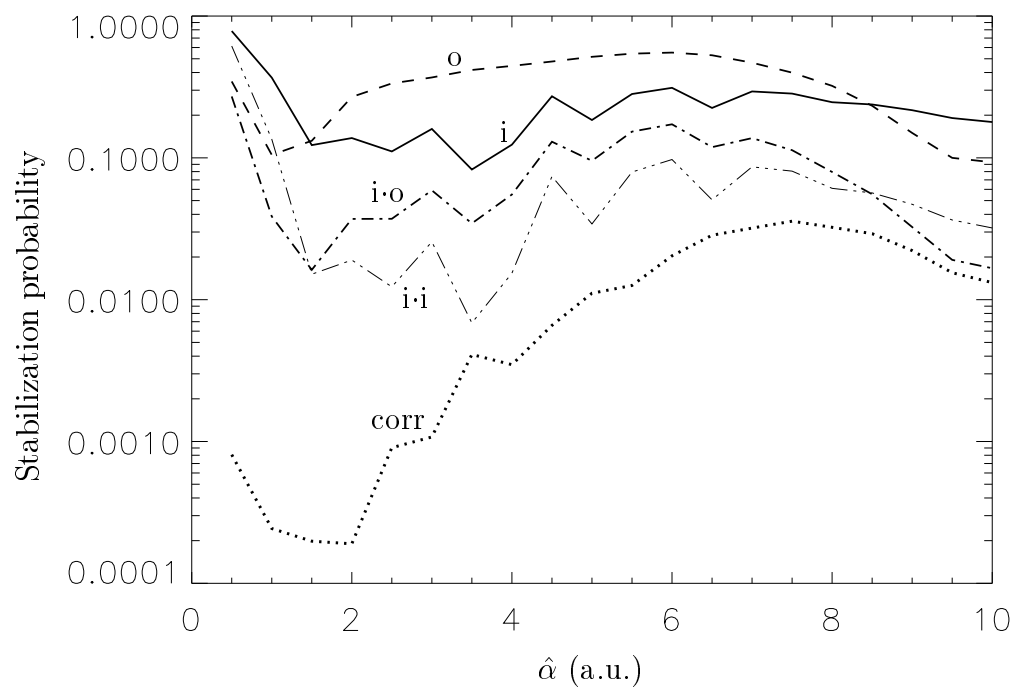


Fig. 7: Bauer and Ceccherini, “Electron correlation vs. ...”

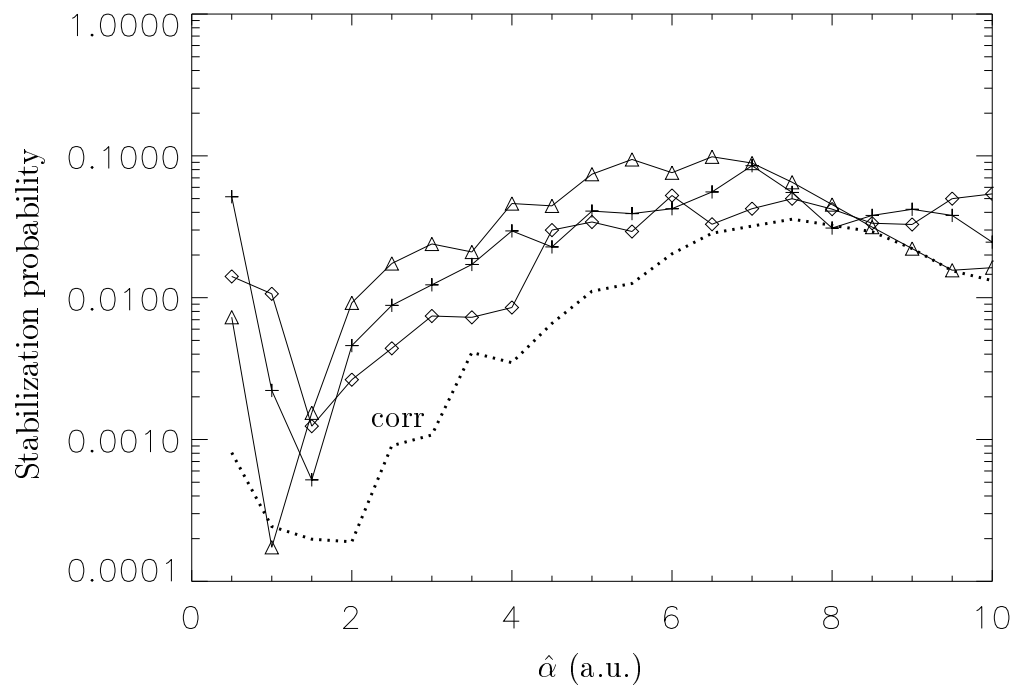


Fig. 8: Bauer and Ceccherini, “Electron correlation vs. ...”